Tunnelling through a Gaussian random barrier

2008 J. Phys. A: Math. Theor. 41 025301

(http://iopscience.iop.org/1751-8121/41/2/025301)

J. Phys. A: Math. Theor. **41** (2008) 025301 (18pp) doi:10.1088/1751-8113/41/2/025301

Tunnelling through a Gaussian random barrier

Viktor Bezák

Department of Experimental Physics, Comenius University, 84248 Bratislava, Slovakia

E-mail: bezak@fmph.uniba.sk

Received 27 June 2007, in final form 14 November 2007
Published 19 December 2007
Online at stacks.iop.org/JPhysA/41/025301

Abstract
A thorough analysis of the tunnelling of electrons through a laterally inhomogeneous rectangular barrier is presented. The barrier height is defined as a statistically homogeneous Gaussian random function. In order to simplify calculations, we assume that the electron energy is low enough in comparison with the mean value of the barrier height. The randomness of the barrier height is defined vertically by a constant variance and horizontally by a finite correlation length. We present detailed calculations of the angular probability density for the tunnelled electrons (i.e. for the scattering forwards). The tunnelling manifests a remarkably diffusive character if the wavelength of the electrons is comparable with the correlation length of the barrier.

PACS numbers: 03.65.−w, 03.65.Nk, 68.49.−h, 73.40.Gk, 73.40.Rw

1. Introduction

As is well known, there exists various quantum-mechanical models of disordered solids. (cf e.g. the well-known monograph [1] where some archetypal approaches to models of disorder were summarized.) One of the fundamental topics with which the theory of disordered solids had ever to cope with was the clarification of the behaviour of electrons in a static field defined by a random potential energy $V(\mathbf{r})$. In the present paper, we intend to show that even the tunnelling problem can be treated with a random potential energy. We define the potential energy in the form

$$V(\mathbf{r}) = [\Theta(z) - \Theta(z-a)]V_0(\vec{\rho}). \tag{1}$$

Here $\vec{\rho} = (x, y)$, $a > 0$ is a small constant and $\Theta(z)$ is the unit step function: $\Theta(z) = 0$ if $z < 0$ and $\Theta(z) = 1$ if $z > 0$. Thus, we assume that the randomness of the potential energy is confined to a thin layer of thickness a. We stipulate that the random function $V_0(\vec{\rho})$ is *stochastically* homogeneous. We assume that the mean value of $V_0(\vec{\rho})$,

$$\langle V_0(\vec{\rho})\rangle = \bar{V}_0 = \text{const} > 0, \tag{2}$$

is sufficiently high. (By the angular brackets $\langle\,\rangle$, we denote the averaging with respect to the randomness of $V_0(\vec{\rho})$.) Outside the layer, the potential energy is equal to zero and so we can consider a particle (say an electron) travelling towards the layer $0 < z < a$ as a plane wave with a given wave vector $\mathbf{k}_0$. The Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + [\Theta(z) - \Theta(z-a)]V_0(\vec{\rho})\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{3}$$

is a stochastic differential equation. Evidently, we may consider the tunnelling as a special problem of the scattering theory. The basic problem is to derive the probability density for the scattering of the electron from the state $|\mathbf{k}_0\rangle$ to an arbitrary state $|\mathbf{k}\rangle$. Since this scattering is elastic, we have to respect that $|\mathbf{k}_0| = |\mathbf{k}| = k$, i.e.

$$\frac{\hbar^2 k_0^2}{2m} = \frac{\hbar^2 k^2}{2m} = E. \tag{4}$$

With a given value of the energy E, we prefer to define the wave vectors $\mathbf{k}_0$ and $\mathbf{k}$ by their directional angles (ϕ_0, θ_0) and (ϕ, θ): $k_x = k\sin\theta\cos\phi$, $k_z = k\cos\theta$, etc. We take $k_{0z} > 0$, i.e. $\theta_0 \in (0, \pi/2)$. We will focus attention on the scattering forwards, i.e. we take $k_z > 0, \theta \in (0, \pi/2)$.

The main objective of the theory presented in this paper is the calculation of the angular probability density $P(\phi, \theta|\phi_0, \theta_0)$ for the scattering $\mathbf{k}_0 \to \mathbf{k}$. In order to exemplify the calculation with a simple, but still relevant, random barrier $V(\mathbf{r})$, we choose $V_0(\vec{\rho})$ as a Gaussian random function with a constant variance

$$\mu^2 = \langle[V_0(\vec{\rho}) - \bar{V}_0]^2\rangle \tag{5}$$

and with the autocorrelation function in the standard form

$$W_0(\vec{\rho}_1; \vec{\rho}_2) = \frac{\langle[V_0(\vec{\rho}_1) - \bar{V}_0][V_0(\vec{\rho}_2) - \bar{V}_0]\rangle}{\mu^2} = \exp\left(-\frac{(\vec{\rho}_1 - \vec{\rho}_2)^2}{2\ell^2}\right). \tag{6}$$

We call the parameter $\ell > 0$ the correlation length of the random barrier $V(\mathbf{r})$. The proper objective of the present paper is to derive the dependence of the tunnelling probability on the energy E and on the three barrier parameters, $\bar{V}_0 > 0$, $\mu \geqslant 0$ and $\ell > 0$.

We focus attention on energy values that are sufficiently low. We stipulate that

$$\mu + \frac{\hbar^2}{2ma^2} < \bar{V}_0 \qquad \text{and} \qquad E < E_{\mathrm{u}}, \tag{7}$$

where

$$E_u = \frac{1}{4}\left(\bar{V}_0 - \mu - \frac{\hbar^2}{2ma^2}\right). \tag{8}$$

E_{u} is meant approximately as the 'upper bound' of the energies that we consider as 'low'. In a typical realization of the Gaussian random function $V_0(\vec{\rho})$, there may exist points $\vec{\rho}$ where $V_0(\vec{\rho})$ is negative and then $V(\mathbf{r})$ is not a barrier but a well at these points. To minimize the occurrence of wells in $V(\mathbf{r})$, we require the variance μ^2 not to be too high, but otherwise we prefer to consider the values of μ as high as possible. As a compromise, we assume that

$$0 < \mu < \min\left\{\bar{V}_0 - \frac{\hbar^2}{2ma^2}, \frac{\bar{V}_0}{4}\right\}. \tag{9}$$

Under this condition, the absolute values of the function

$$v_0(\vec{\rho}) = V_0(\vec{\rho}) - \bar{V}_0 \tag{10}$$

at most points $\vec{\rho}$ are small in comparison with $\bar{V}_0$. Owing to this fact, we can simplify some expressions in our calculations. In particular, we may use the approximation

$$\sqrt{V_0(\vec{\rho}) - E} \approx \sqrt{\bar{V}_0 - E} - \frac{v_0(\vec{\rho})}{2\sqrt{\bar{V}_0 - E}}. \tag{11}$$

If $\mu = 0$, the barrier is homogeneous. This case is deterministic. The theory of the tunnelling in this case is well-known (cf e.g. [2]). If $\ell \to \infty$ and $\mu > 0$, the problem is not deterministic, but we can interpret $\langle\,\rangle$ as the averaging over a statistical ensemble of homogeneous barriers. Our intent, however, is to solve the tunnelling problem in the general case when $\mu > 0$ and when the correlation length $\ell > 0$ is finite.

We address the present paper mainly to theorists, since the problem under consideration is interesting from a quantum-mechanical viewpoint in its own right. On the other hand, evidently the problem is also of interest in view of some microelectronic applications.

2. 1D case: tunnelling through a rectangular barrier

If $\mu = 0$ but also if $\mu > 0$ and $\ell \to \infty$, the wavefunctions are factorized as $\psi(\mathbf{r}) = \exp[\mathrm{i}(k_x x + k_y y)]\psi_{1\mathrm{D}}(z)$ so that we may confine ourselves to discussing the 1D case.

2.1. Single barrier

The tunnelling concerns energies $E < V_0$. If a particle of mass $m > 0$ impacts upon the barrier from the left, we write

$$k = k_z = \frac{\sqrt{2mE}}{\hbar}, \qquad \kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}. \tag{12}$$

We obtain easily the reflection coefficient

$$\mathcal{R}(V_0) = |A|^2 = \frac{(\kappa^2 + k^2)^2 \sinh^2(\kappa a)}{(\kappa^2 + k^2)^2 \sinh^2(\kappa a) + 4\kappa^2 k^2} \tag{13}$$

and the transmission coefficient

$$\mathcal{T}(V_0) = |A|^2 = \frac{4\kappa^2 k^2}{(\kappa^2 + k^2)^2 \sinh^2(\kappa a) + 4\kappa^2 k^2}. \tag{14}$$

Clearly, $\mathcal{R}(V_0) + \mathcal{T}(V_0) = 1$. If $\kappa a \gg 1$, i.e. if $V_0 - E \gg \hbar^2/(2ma^2)$, the tunnelling probability can be approximated as

$$\mathcal{T}(V_0) \approx 16\left(1 - \frac{E}{V_0}\right)\frac{E}{V_0}\exp\left(-\frac{2a\sqrt{2m(V_0 - E)}}{\hbar}\right). \tag{15}$$

2.2. Gaussian ensemble of barriers with random height

Let us now assume that V_0 is a Gaussian random variable. We consider a Gaussian ensemble of barriers. The probability to find a barrier with the height in the interval $(V_0, V_0 + \mathrm{d}V_0)$ in this ensemble is equal to $P_{\mathrm{G}}(V_0)\,\mathrm{d}V_0$ where

$$P_{\mathrm{G}}(V_0) = \frac{1}{\sqrt{2\pi\mu^2}}\exp\left(-\frac{(V_0 - \bar{V}_0)^2}{2\mu^2}\right) = \frac{1}{\sqrt{2\pi\mu^2}}\exp\left(-\frac{v_0^2}{2\mu^2}\right). \tag{16}$$

(cf equation (10).) The function $1/V_0$ in the factor in front of the exponential in formula (15) can be written as $1/V_0 \approx 1/\bar{V}_0(1 - v_0/\bar{V}_0)$. Hence

$$\left(1 - \frac{E}{V_0}\right)\frac{1}{V_0} \approx \left(1 - \frac{E}{\bar{V}_0}\right)\frac{1}{\bar{V}_0} - \left(1 - \frac{2E}{\bar{V}_0}\right)\frac{v_0}{\bar{V}_0^2} + \cdots \tag{17}$$

We accept the approximation

$$\exp\left(-\frac{2a\sqrt{2m(V_0-E)}}{\hbar}\right)\approx\exp\left(-\frac{2a\sqrt{2m(\bar{V}_0-E)}}{\hbar}\right)\exp\left(-\frac{a}{\hbar}\sqrt{\frac{2m}{\bar{V}_0-E}}v_0\right). \tag{18}$$

The proper objective of this subsection is the calculation of the mean value

$$\langle\mathcal{T}\rangle=\int_{-\infty}^{\infty}\mathrm{d}V_0\mathcal{T}(V_0)P_\mathrm{G}(V_0). \tag{19}$$

In regard to formula (17), we write

$$\langle\mathcal{T}\rangle\approx\langle\mathcal{T}_0\rangle+\langle\mathcal{T}_1\rangle. \tag{20}$$

The first (second) term in this formula corresponds to the first (second) term on the rhs of expression (17). We will now derive the condition under which the term $\langle\mathcal{T}_1\rangle$ is much smaller than the term $\langle\mathcal{T}_0\rangle$

$$\langle\mathcal{T}_0\rangle=\bar{\mathcal{T}}\exp\left(\frac{ma^2\mu^2}{\hbar^2(\bar{V}_0-E)}\right). \tag{21}$$

Here

$$\bar{\mathcal{T}}=\mathcal{T}(\bar{V}_0)\approx 16\left(1-\frac{E}{\bar{V}_0}\right)\frac{E}{\bar{V}_0}\exp\left(-\frac{2a\sqrt{2m(\bar{V}_0-E)}}{\hbar}\right). \tag{22}$$

Since we are discussing the case when $\hbar^2/(2ma^2)\ll\bar{V}_0$, we choose the upper bound of the values of μ for which the approximations used in the present paper may apply as $\mu_\mathrm{u}=\bar{V}_0/4$ (cf inequality (9)) and the value of E_u, defined by expression (8), as $(\bar{V}_0-\mu_\mathrm{u})/4=3\bar{V}_0/16$. When inserting μ_u for μ and E_u for E in the exponent of the exponential of expression (21), we obtain the value

$$\frac{m\mu_\mathrm{u}^2a^2}{\hbar^2(\bar{V}_0-E_\mathrm{u})}=\frac{2}{13}\left(\frac{2ma^2}{\hbar^2}\right)\bar{V}_0. \tag{23}$$

This value can be relatively high and so the exponential factor in formula (21) can become considerably—even by the order of magnitude—greater than unity.

We can calculate the term

$$\langle\mathcal{T}_1\rangle=-\bar{\mathcal{T}}\frac{1}{\bar{V}_0}\left[\left(1-\frac{2E}{\bar{V}_0}\right)\Big/\left(1-\frac{E}{\bar{V}_0}\right)\right]\int_{-\infty}^{\infty}\mathrm{d}v_0\,v_0\exp\left(\frac{a}{\hbar}\sqrt{\frac{2m}{\bar{V}_0-E}}v_0\right)P_\mathrm{G}(V_0)$$

without resorting to numerical computations:

$$\langle\mathcal{T}_1\rangle=-\sqrt{\frac{2ma^2}{\hbar^2}}\frac{(\bar{V}_0-2E)\mu^2}{\bar{V}_0(\bar{V}_0-E)^{3/2}}\langle\mathcal{T}_0\rangle. \tag{24}$$

Therefore, we may state that $|\langle\mathcal{T}_1\rangle|\ll\langle\mathcal{T}_0\rangle$ if

$$\frac{(\bar{V}_0-2E)^2\mu^4}{\bar{V}_0(\bar{V}_0-E)^3}\ll\frac{\hbar^2}{2ma^2}. \tag{25}$$

The lhs of this inequality can be much smaller than $\bar{V}_0$ even with relatively high values of μ. Indeed, the substitution of μ_u and E_u for μ and E, respectively, gives us the value $(\bar{V}_0-2E_\mathrm{u})^2\mu_\mathrm{u}^4/[\bar{V}_0(\bar{V}_0-E_\mathrm{u})^3]\approx 0.003\bar{V}_0$. Thus we may conclude that

$$\langle\mathcal{T}\rangle\approx\langle\mathcal{T}_0\rangle\qquad\text{if}\quad\frac{\hbar^2}{2ma^2}>0.01\bar{V}_0. \tag{26}$$

For $\hbar^2/(2ma^2) = 0.01\bar{V}_0$, $\mu = \bar{V}_0/4$ and $E = 3\bar{V}_0/16$, we find that

$$\exp\left(\frac{ma^2\mu^2}{\hbar^2(\bar{V}_0 - E)}\right) = \exp(50/13) \approx 47,$$

so that we may state that, according to formula (21), the mean value $\langle \mathcal{T} \rangle$ may be as much as fifty times higher than the tunnelling probability $\bar{\mathcal{T}}$ calculated for the corresponding deterministic barrier with $V_0 \equiv \bar{V}_0$.

The enhancement of the tunnelling probability as a consequence of the Gaussian randomness of V_0 is comprehensible. If the correlation length ℓ is large, there are wide areas on the barrier plane $z = 0$ where V_0 is almost constant. However, the value of V_0 varies from area to area. The electron prefers to tunnel through areas where V_0 is lower than $\bar{V}_0$.

3. 3D case: tunnelling through a narrow inhomogeneous rectangular barrier (mathematical formulation of the problem)

In this section, we will follow the general method that we recently applied when examining the problem of the tunnelling through an inhomogeneous delta-barrier [3, 4]. In the present paper, we want to show how this method works in the case of the tunnelling through an inhomogeneous rectangular barrier of a non-zero thickness a. We assume that the value of $a > 0$ is small in comparison with ℓ, and that $|\partial \ln V_0(\vec{\rho})/\partial x|\ell \ll 1$, $|\partial \ln V_0(\vec{\rho})/\partial y|\ell \ll 1$.

3.1. General solution of the Schrödinger equation with an arbitrary function $V_0(\vec{\rho})$

Let us now consider the de Broglie wave $\exp(\mathrm{i}\mathbf{k}_0 \cdot \mathbf{r})$ impacting upon the plane $z = 0$ with $k_{0z} > 0$. This wave is scattered on the barrier both backwards and forwards. We will use the denotation

$$\psi(\mathbf{r}) = \begin{cases} \exp(\mathrm{i}\mathbf{k}_0 \cdot \mathbf{r}) + F_1(\mathbf{r}) & \text{if} \quad z < 0, \\ F_2(\mathbf{r}) & \text{if} \quad z > a. \end{cases} \tag{27}$$

Let us imagine a straight line intersecting perpendicularly the plane $z = 0$ in a point $\mathbf{r}_1 = (\vec{\rho}, 0)$ and correspondingly the plane $z = a$ in the point $\mathbf{r}_2 = (\vec{\rho}, a)$. In the close vicinity of these two points, we may take $V_0(\vec{\rho})$ as a constant. Thus we write

$$\begin{aligned} F_1(\mathbf{r}) &\approx A(\vec{\rho}) \exp[\mathrm{i}(k_{0x}x + k_{0y}y)] \exp(-\mathrm{i}k_{0z}z)], \qquad z < 0, \\ F_2(\mathbf{r}) &\approx C(\vec{\rho}) \exp[\mathrm{i}(k_{0x}x + k_{0y}y)] \exp(\mathrm{i}k_{0z}z), \qquad z > a. \end{aligned} \tag{28}$$

Using the continuity of $\psi(\mathbf{r})$ and of $\partial\psi(\mathbf{r})/\partial z$, we obtain the coefficients

$$A(\vec{\rho}) = -\frac{\left[\kappa_z(\vec{\rho})^2 + k_{0z}^2\right]\{\exp[\kappa_z(\vec{\rho})a] - \exp[-\kappa_z(\vec{\rho})a]\}}{[\kappa_z(\vec{\rho}) - \mathrm{i}k_{0z}]^2 \exp[\kappa_z(\vec{\rho})a] - [\kappa_z(\vec{\rho}) + \mathrm{i}k_{0z}]^2 \exp[-\kappa_z(\vec{\rho})a]}, \tag{29}$$

$$C(\vec{\rho}) = -\frac{4\mathrm{i}\kappa_z(\vec{\rho})k_{0z} \exp(-\mathrm{i}k_{0z}a)}{[\kappa_z(\vec{\rho}) - \mathrm{i}k_{0z}]^2 \exp[\kappa_z(\vec{\rho})a] - [\kappa_z(\vec{\rho}) + \mathrm{i}k_{0z}]^2 \exp[-\kappa_z(\vec{\rho})a]}, \tag{30}$$

with

$$\kappa_z(\vec{\rho}) = \sqrt{2mV_0(\vec{\rho})/\hbar^2 - k_{0z}^2}. \tag{31}$$

Respecting expressions (28), we obtain the locally given functions

$$\left.\frac{\partial F_1(\mathbf{r})}{\partial z}\right|_{z=-0} = -\mathrm{i}k_{0z}A(\vec{\rho}), \qquad \left.\frac{\partial F_2(\mathbf{r})}{\partial z}\right|_{z=a+0} = \mathrm{i}k_{0z}C(\vec{\rho}). \tag{32}$$

If the function $V_0(\vec{\rho})$ is random, this implies that the function $\kappa_z(\vec{\rho})$ is random and, consequently, also the functions $A(\vec{\rho})$ and $C(\vec{\rho})$ are random.

Equation (3) can be solved by Kirchhoff's method. We have to employ Green's function of the problem. We define separately Green's function for $z < 0$ and for $z > a$:

$$\begin{aligned} G_1(\mathbf{r}|\mathbf{r}_0) &= G_0(\vec{\rho}, z|\vec{\rho}_0, z_0) + G_0(\vec{\rho}, z|\vec{\rho}_0, -z_0) \qquad \text{for} \quad z < 0, \\ G_2(\mathbf{r}|\mathbf{r}_0) &= G_0(\vec{\rho}, z-a|\vec{\rho}_0, z_0 - a) + G_0(\vec{\rho}, z-a|\vec{\rho}_0, -z_0 + a) \qquad \text{for} \quad z > a. \end{aligned} \tag{33}$$

Here

$$G_0(\mathbf{r}|\mathbf{r}_0) = \frac{\exp(\mathrm{i}k|\mathbf{r}-\mathbf{r}_0|)}{4\pi|\mathbf{r}-\mathbf{r}_0|}, \qquad k = k_0 = \frac{\sqrt{2mE}}{\hbar}. \tag{34}$$

We have chosen the symmetrized form of the functions $G_1(\mathbf{r}|\mathbf{r}_0)$ and $G_2(\mathbf{r}|\mathbf{r}_0)$ in order to utilize the zero value of their normal derivatives:

$$\left.\frac{\partial G_1(\mathbf{r}|\mathbf{r}_0)}{\partial z}\right|_{z=-0} = 0, \qquad \left.\frac{\partial G_2(\mathbf{r}|\mathbf{r}_0)}{\partial z}\right|_{z=a+0} = 0. \tag{35}$$

Owing to the first of these equalities, we can express quite generally the function $F_1(\mathbf{r})$ by the formula

$$\begin{aligned} F_1(\mathbf{r}) &= \int \mathrm{d}^2\rho' G_1(\vec{\rho}', 0|\mathbf{r}) \left.\frac{\partial F_1(\mathbf{r}')}{\partial z'}\right|_{z'=-0} \\ &= \frac{1}{2\pi}\int \mathrm{d}^2\rho' \frac{\exp\left(\mathrm{i}k\sqrt{(\vec{\rho}'-\vec{\rho})^2+z^2}\right)}{\sqrt{(\vec{\rho}'-\vec{\rho})^2+z^2}} \left.\frac{\partial F_1(\mathbf{r}')}{\partial z'}\right|_{z'=-0}, \qquad z < 0. \end{aligned} \tag{36a}$$

Similarly we may write

$$\begin{aligned} F_2(\mathbf{r}) &= -\int \mathrm{d}^2\rho' G_2(\vec{\rho}', a|\mathbf{r}) \left.\frac{\partial F_2(\mathbf{r}')}{\partial z'}\right|_{z'=a+0} \\ &= -\frac{1}{2\pi}\int \mathrm{d}^2\rho' \frac{\exp\left(\mathrm{i}k\sqrt{(\vec{\rho}'-\vec{\rho})^2+(z-a)^2}\right)}{\sqrt{(\vec{\rho}'-\vec{\rho})^2+(z-a)^2}} \left.\frac{\partial F_2(\mathbf{r}')}{\partial z'}\right|_{z'=a+0}, \qquad z > 0. \end{aligned} \tag{36b}$$

3.2. Deterministic function $V_0(\vec{\rho})$: approximation for energies $\hbar^2 k_{0z}^2/(2m)$ that are much lower than the minimum of $V_0(\vec{\rho})$

Let $V_0(\vec{\rho})$ be an arbitrary positive function and let $V_0^{\min} > 0$ be its minimum value. Respecting formula (31), we define the parameter $\kappa_z^{\min} = \sqrt{2mV_0^{\min}/\hbar^2 - k_{0z}^2}$. We stipulate the fulfilment of the condition $\kappa_z^{\min} a \gg 1$, i.e.

$$V_0^{\min} \gg \frac{\hbar^2}{2m}\left(\frac{1}{a^2} + k_{0z}^2\right). \tag{37}$$

Under this condition, expressions (29) and (30) become much simpler:

$$A(\vec{\rho}) \approx \frac{\kappa_z(\vec{\rho})^2 + k_{0z}^2}{[\kappa_z(\vec{\rho}) - \mathrm{i}k_{0z}]^2}, \qquad C(\vec{\rho}) \approx -\frac{4\mathrm{i}\kappa_z(\vec{\rho})k_{0z}}{[\kappa_z(\vec{\rho}) - \mathrm{i}k_{0z}]^2}\exp\{-[\kappa_z(\vec{\rho}) + \mathrm{i}k_{0z}]a\}. \tag{38}$$

3.3. Low-energy approximation with the Gaussian random function $V_0(\vec{\rho})$

If $V_0(\vec{\rho})$ is defined as a Gaussian random function, condition (37) cannot be applied. Instead, we require the fulfilment of the conditions

$$0 < \mu < \mu_{\mathrm{u}}, \qquad 0 < k_{0z} < k_{\mathrm{u}}, \tag{39}$$

where $\mu_{\rm u} = \bar{V}_0/4$ and where $k_{\rm u}$ is defined by the equation $E_{\rm u} = \hbar^2 k_{\rm u}^2/(2m) = (\bar{V}_0 - \mu_{\rm u})/4 = 3\bar{V}_0/16$. (Here we have taken into account, with a minor modification respecting the 3D case, what we have discussed in subsection 2.2 in the 1D case.) Employing the function $v_0(x, y)$ (cf expression (10)), we can write

$$\kappa_z(\vec{\rho}) = \bar{\kappa}_z \sqrt{1 + \frac{2m}{\hbar^2 \bar{\kappa}_z^2} v_0(\vec{\rho})}, \qquad \bar{\kappa}_z = \sqrt{\frac{2m\bar{V}_0}{\hbar^2} - k_{0z}^2}. \tag{40}$$

Since μ is small in comparison with $E_{\rm u}$ and $\bar{V}_0 - E_{\rm u}$, we may use the development

$$\kappa_z(\vec{\rho}) = \bar{\kappa}_z \left[1 + \frac{m}{\hbar^2 \bar{\kappa}_z^2} v_0(\vec{\rho}) - \frac{1}{2} \left(\frac{m}{\hbar^2 \bar{\kappa}_z^2} \right)^2 [v_0(\vec{\rho})]^2 + \cdots \right]. \tag{41}$$

Then also

$$A(\vec{\rho}) = \bar{A} + A_1 v_0(\vec{\rho}) + A_2 [v_0(\vec{\rho})]^2 + \cdots \tag{42}$$

($\bar{A}$ is the value of $A(\vec{\rho})$ if $V_0(\vec{\rho})$ is substituted by $\bar{V}_0$.) Similarly we can write

$$-\frac{4{\rm i}\kappa_z(\vec{\rho})k_{0z}}{[\kappa_z(\vec{\rho}) - {\rm i}k_{0z}]^2} \approx -\frac{4{\rm i}\bar{\kappa}_z k_{0z}}{[\bar{\kappa}_z - {\rm i}k_{0z}]^2} + C_1 v_0(\vec{\rho}) + C_2 [v_0(\vec{\rho})]^2 + \cdots \tag{43}$$

By analogy with expression (18), we accept the exponential with the exponent in the linear approximation with respect to $v_0(\vec{\rho})$:

$$\exp\{-[\kappa_z(\vec{\rho}) + {\rm i}k_{0z}]a\} \approx \exp[-(\bar{\kappa}_z + {\rm i}k_{0z})a] \exp\left(-\frac{ma}{\hbar^2 \bar{\kappa}_z} v_0(\vec{\rho}) \right). \tag{44}$$

When utilizing formulae (32), (36*a*) and (36*b*), we can readily calculate averaged functions like $\langle |F_\alpha(\mathbf{r})|^2 \rangle$ or $\langle F_\alpha(\mathbf{r}) \nabla F_\alpha^*(\mathbf{r}) \rangle$, $\alpha = 1, 2$. The value of $\bar{A}$ determines the probability of the regular reflection from the barrier and the coefficients $A_1, A_2, \ldots$ determine the diffusive character of the backscattering. However, the backscattering is not the proper topic of the present paper. We note only that when the parameter μ is small, the influence of the barrier randomness on the reflection of low-energy electrons is weak.

We focus attention on the forward scattering. Assuming that the value of $\hbar^2/(2ma^2)$ may be greater than $0.01\bar{V}_0$, say, we may neglect the terms with $C_1, C_2, \ldots$ in series (43). Employing formula (42.2) in this approximation, we express the function $F_2(\mathbf{r})$ as

$$F_2(\mathbf{r}) \approx -\frac{2\bar{\kappa}_z k_{0z}^2}{\pi [\bar{\kappa}_z - {\rm i}k_{0z}]^2} \exp[-(\bar{\kappa}_z + {\rm i}k_{0z})a] I(\vec{\rho}), \tag{45}$$

where

$$I(\vec{\rho}) = \int {\rm d}^2\rho' \exp[{\rm i}(k_{0x}x' + k_{0y}y')] \frac{\exp({\rm i}k\sqrt{(\vec{\rho}' - \vec{\rho})^2 + (z-a)^2})}{\sqrt{(\vec{\rho}' - \vec{\rho})^2 + (z-a)^2}} \exp\left(-\frac{mav_0(\vec{\rho}')}{\hbar^2 \bar{\kappa}_z} \right).$$

Since our intention is to treat the tunnelling as a specific problem of the scattering theory, we prefer to pay heed on the asymptotic behaviour of the function $F_2(\mathbf{r})$, i.e. for

$$kz \gg 1, \qquad z \gg a. \tag{46}$$

Under these conditions, we may use the approximation

$$\frac{\exp[{\rm i}k\sqrt{(\vec{\rho}' - \vec{\rho})^2 + z^2}]}{\sqrt{(x'-x)^2 + (y'-y)^2 + z^2}} \approx \frac{\exp({\rm i}kR)}{R} \exp\left(-{\rm i}k \frac{xx' + yy'}{R} \right), \qquad R = |\mathbf{r}|. \tag{47}$$

Then $I(\vec{\rho})$ turns into the Fourier integral:

$$I(\vec{\rho}) \approx \frac{\exp({\rm i}kR)}{R} \int {\rm d}^2\rho' \exp\left\{ {\rm i}\left[\left(k_{0x} - \frac{kx}{R} \right) x' + \left(k_{0y} - \frac{ky}{R} \right) y' \right] \right\} \exp\left(-\frac{mav_0(\vec{\rho}')}{\hbar^2 \bar{\kappa}_z} \right). \tag{48}$$

4. Angular distribution of the tunnelling into a given direction

Let us realize a square diaphragm attached to the plane $z = 0$ so that the tunnelling may be allowed through the opening $\Box$ defined by the inequalities $-L/2 < x < L/2$ and $-L/2 < y < L/2$. If $z = R\cos\Theta \to \infty$, we may state that $|x| \gg L/2$ and $|y| \gg L/2$ for almost all values of $\Theta \in (0, \pi/2)$ (except for values of Θ approaching zero). Moreover, we require that L may be large enough in comparison with the correlation length ℓ of the random function $v_0(x, y)$:

$$0 < \ell \ll L \ll z. \tag{49}$$

Since an observer standing at any distant point $\mathbf{r}$ sees the square $L \times L \equiv \Box$ as an almost point-like object, we may state that the function $\langle |F_2(\mathbf{r})|^2\rangle$, if considered on a hemisphere $|\mathbf{r}| = R = \text{const}$, maps the angular distribution of the tunnelling probability. Therefore, we will calculate the integral

$$|I_\Box(\vec{\rho})|^2 = (1/R^2)\int_\Box \mathrm{d}^2\rho' \int_\Box \mathrm{d}^2\rho'' \times \exp\left\{\mathrm{i}\left[\left(k_{0x} - \frac{kx}{R}\right)(x' - x'') + \left(k_{0y} - \frac{ky}{R}\right)(y' - y'')\right]\right\}\mathcal{F}\{v_0(\tilde{\vec{\rho}})\}, \tag{50}$$

with the functional

$$\mathcal{F}\{v_0(\tilde{\vec{\rho}})\} = \exp\left(-\frac{ma[v_0(\vec{\rho}') + v_0(\vec{\rho}'')]}{\hbar^2\bar{\kappa}_z}\right). \tag{51}$$

Integral (50) is proportional to L^2, so we define the function

$$\varphi(\vec{\rho}|\mathbf{k}_0) = \lim_{L\to\infty} |I_\Box(\vec{\rho})|^2/L^2. \tag{52}$$

Functional (51) can be written in the form $\mathcal{F}\{v_0(\tilde{\vec{\rho}})\} = \exp\left[-\int \mathrm{d}^2\tilde{\rho}\, \beta(\tilde{\vec{\rho}})v_0(\tilde{\vec{\rho}})\right]$ with $\beta(\tilde{\vec{\rho}}) = [ma/(\hbar^2\bar{\kappa}_z)][\delta(\tilde{\vec{\rho}} - \vec{\rho}') + \delta(\tilde{\vec{\rho}} - \vec{\rho}'')]$. The Gaussian random function $v_0(\vec{\rho})$ is zero-centered. With an arbitrary function $\beta(\tilde{\vec{\rho}})$, we may use the general formula

$$\left\langle \exp\left[-\int \mathrm{d}^2\tilde{\rho}\, \beta(\tilde{\vec{\rho}})v_0(\tilde{\vec{\rho}})\right]\right\rangle = \exp\left(\frac{\mu^2}{2}\iint \mathrm{d}^2\tilde{\rho}'\,\mathrm{d}^2\tilde{\rho}''\beta(\tilde{\vec{\rho}}')W_0(\tilde{\vec{\rho}}'; \tilde{\vec{\rho}}'')\beta(\tilde{\vec{\rho}}'')\right), \tag{53}$$

where W_0 is the autocorrelation function of $v_0(\vec{\rho})$. (cf definition (6).) (At another occasion, we used already formula (53) with $\beta = \text{const}$ in our early paper [5].) Employing formula (53), we can readily derive the function

$$\langle \mathcal{F}\{v_0(\tilde{x}, \tilde{y})\}\rangle = \exp\{u^2[1 + W_0(x', y'; x'', y'')]\}, \tag{54}$$

where

$$u = \frac{ma\mu}{\hbar^2\bar{\kappa}_z}. \tag{55}$$

In the 1D case (i.e. when $k_{0x} = k_{0y} = 0$), the value of u^2 would be equal to $ma^2\mu^2/[\hbar^2(\bar{V}_0 - E)]$. This value can be (as we have shown in subsection 2.2) comparable with unity even if the value of μ is small.

It is convenient to use the variables $\xi = x' - x''$, $\eta = y' - y''$ and $X = \frac{1}{2}(x' + x'')$, $Y = \frac{1}{2}(y' + y'')$. Then we easily find that

$$\varphi(\vec{\rho}|\mathbf{k}_0) = \frac{\exp(u^2)}{R^2}\chi(\vec{\rho}|\mathbf{k}_0), \tag{56}$$

where

$$\chi(\vec{\rho}|\mathbf{k}_0) = \int_{-\infty}^{\infty}\mathrm{d}\xi\int_{-\infty}^{\infty}\mathrm{d}\eta\,\exp\left\{\mathrm{i}\left[\left(k_{0x} - \frac{kx}{R}\right)\xi + \left(k_{0y} - \frac{ky}{R}\right)\eta\right]\right\}\exp[u^2W_0(\sqrt{\xi^2 + \eta^2})].$$

Here we have preferred to write $W_0(\sqrt{\xi^2+\eta^2})$ instead of $W_0(x', y'; x'', y'')$. Using the series

$$\exp\left[u^2 \exp\left(-\frac{\xi^2+\eta^2}{2\ell^2}\right)\right] = \sum_{n=0}^{\infty} \frac{u^{2n}}{n!} \exp\left(-n\frac{\xi^2+\eta^2}{2\ell^2}\right),$$

we may consider the sum

$$\chi(\vec{\rho}|\mathbf{k}_0) = \chi^0(\vec{\rho}|\mathbf{k}_0) + \sum_{n=1}^{\infty} \chi_n(\vec{\rho}|\mathbf{k}_0), \tag{57}$$

so that

$$\frac{1}{(2\pi)^2}\chi^0(\vec{\rho}|\mathbf{k}_0) = \delta\left(k_{0x} - \frac{kx}{R}\right)\delta\left(k_{0y} - \frac{ky}{R}\right)$$

and

$$\frac{1}{(2\pi)^2}\chi_n(\vec{\rho}|\mathbf{k}_0) = \frac{u^{2n}}{n!}\frac{\ell^2}{2\pi n}\exp\left[-\frac{\ell^2}{2n}\left[\left(k_{0x} - \frac{kx}{R}\right)^2 + \left(k_{0y} - \frac{ky}{R}\right)^2\right]\right], \qquad n \geqslant 1.$$

Evidently,

$$\chi^\infty(\vec{\rho}|\mathbf{k}_0) = \exp(u^2)\chi^0(\vec{\rho}|\mathbf{k}_0). \tag{58}$$

The superscripts 0 and ∞ mean (and in other functions will also mean) that the correlation length ℓ is taken either as zero or as infinity. If ℓ is finite, this implies a certain diffusive character of the tunnelling. Since the functions $\chi^0(\vec{\rho}|\mathbf{k}_0)$ and $\chi_n(\vec{\rho}|\mathbf{k}_0)$ concern an arbitrary point $\mathbf{r}$ located far away from the barrier, we can imagine a ray emitted from the center of the square $L \times L$ to $\mathbf{r}$ and characterize this ray by the wave vector $\mathbf{k} = k\mathbf{r}/R$. (Recall that $R = |\mathbf{r}|$.) Using the directional angles ϕ, θ and ϕ_0, θ_0 of the vectors $\mathbf{k}$ and $\mathbf{k}_0$, respectively, we identify the product $\delta(k_x - k_{0x})\delta(k_y - k_{0y})\delta(k_z - k_{0z})$ with

$$\delta(\mathbf{k} - \mathbf{k}_0) = \frac{1}{k^2 \sin\theta}\delta(k - k_0)\delta(\phi - \phi_0)\delta(\theta - \theta_0).$$

The factor $\delta(k - k_0)$ is due to the conservation of energy. (We have abandoned this factor in our definition of the functions $\chi_n(\vec{\rho}|\mathbf{k}_0)$, keeping the values of $|\mathbf{k}|$ *a priori* constant.)

To derive the angular distribution of the tunnelling probability, we define the scattering matrix

$$S(\phi, \theta|\phi_0, \theta_0) = \left(\frac{k}{2\pi}\right)^2 \tilde{Q}(k, \theta_0)\exp(u^2)\chi(x, y|\mathbf{k}_0). \tag{59}$$

In agreement with (57), we write the series

$$S(\phi, \theta|\phi_0, \theta_0) = S^0(\phi, \theta|\phi_0, \theta_0) + \sum_{n=1}^{\infty} S_n(\phi, \theta|\phi_0, \theta_0) \tag{60}$$

with the terms

$$S^0(\phi, \theta|\phi_0, \theta_0) = \frac{\tilde{Q}(k, \theta_0)}{\sin\theta}\exp(u^2)\delta(\phi - \phi_0)\delta(\theta - \theta_0) \tag{61}$$

and

$$\begin{aligned} S_n(\phi, \theta|\phi_0, \theta_0) &= \tilde{Q}(k, \theta_0)\exp(u^2)\frac{u^{2n}}{n!}\frac{k^2\ell^2}{2\pi n} \\ &\quad \times \exp\left[-\frac{k^2\ell^2}{2n}(\sin^2\theta_0 - 2\sin\theta_0\sin\theta\cos(\phi - \phi_0) + \sin^2\theta)\right], \qquad n \geqslant 1. \end{aligned} \tag{62}$$

The factor $\tilde{Q}(k, \theta_0)$ depends, in addition to k and θ_0, on the parameters defining the barrier. The Gaussian random barrier treated in the present paper has been defined with four parameters: the thickness a, the mean height $\bar{V}_0$, the variance μ^2 and the correlation length ℓ. In fact, the parameters a, $\bar{V}_0$ and μ form together the parameter u (cf expression (55)). The parameter μ, and then also u, characterizes the 'vertical uncertainty' of the barrier height $V_0(\vec{\rho})$. (Recall that μ is the r.m.s. of $V_0(\vec{\rho})$.) Expression (62) involves also another dimensionless parameter, namely

$$w = k\ell. \tag{63}$$

This parameter characterizes the 'horizontal randomness' of $V_0(\vec{\rho})$: if $1/k$ is chosen as the unit length, w may be interpreted as a characteristic width of the random undulation of the function $V_0(\vec{\rho})$. If the value of w is low (high), the random undulation of $V_0(\vec{\rho})$ around the mean value $\bar{V}_0$ is rapid (slow) in any direction parallel with the plane of the barrier. The factor $\tilde{Q}(k, \theta_0)$, being a function of the parameter u, does not vary with the parameter w. This is because the dependence on ℓ is entirely absorbed in the function $\chi(\vec{\rho}|\mathbf{k}_0)$. That is why

$$\tilde{Q}(k, \theta_0)\exp(u^2) \equiv Q(u, \mathbf{k}_0)\exp(u^2) = \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi/2} \mathrm{d}\theta \, \sin\theta \, S^0(\phi, \theta|\phi_0, \theta_0). \tag{64}$$

As the probability of the tunnelling through a planar barrier is always related to the normal component of the velocity of the impacting particles, we multiply expression (64) by $\cos\theta_0$ and obtain the equality $\cos\theta_0 Q(u, \mathbf{k}_0)\exp(u^2) = \mathcal{T}(u, \mathbf{k}_0) = \bar{\mathcal{T}}(k, \theta_0)\exp(u^2)$. Thus, $\cos\theta_0 Q(u, \mathbf{k}_0) = \bar{\mathcal{T}}(u, \mathbf{k}_0)$ and

$$\mathcal{T}^\infty(u, \mathbf{k}_0) = \mathcal{T}^0(u, \mathbf{k}_0)\exp(u^2) = \bar{\mathcal{T}}(u, \mathbf{k}_0)\exp(2u^2) = \bar{\mathcal{T}}(k, \theta_0)\exp(u^2). \tag{65}$$

The symbol $\bar{\mathcal{T}}(k, \theta_0)$ signifies the 3D analogue to expression (22):

$$\begin{aligned}\bar{\mathcal{T}}(k, \theta_0) &\approx 16\frac{\bar{\kappa}_z^2 k_{0z}^2}{\left(\bar{\kappa}_z^2 + k_{0z}^2\right)^2}\exp(-2a\bar{\kappa}_z) \\ &= 16\frac{\hbar^2 k^2 \cos^2\theta_0}{2m\bar{V}_0}\left(1 - \frac{\hbar^2 k^2\cos^2\theta_0}{2m\bar{V}_0}\right)\exp\left(-2a\sqrt{\frac{2m\bar{V}_0}{\hbar^2} - k^2\cos^2\theta_0}\right).\end{aligned} \tag{66}$$

The value of $\bar{\mathcal{T}}(k, \theta_0)$ would mean the tunnelling probability if the barrier of thickness a were homogeneous with the height equal to $\bar{V}_0$. Note that the parameter u itself depends on the angle of incidence θ_0:

$$u^2 = \left(\frac{ma\mu}{\hbar^2}\right)^2 \Big/ \left(\frac{2m\bar{V}_0}{\hbar^2} - k^2\cos^2\theta_0\right).$$

5. Diffusivity of the tunnelling

5.1. Dependence of the tunnelling probability upon the correlation length ℓ of the random barrier height

We introduce the functions

$$\sigma^0(\theta|\theta_0) = \int_{-\pi}^{\pi} \mathrm{d}\phi \, S^0(\phi, \theta|\phi_0, \theta_0), \qquad \sigma_n(\theta|\theta_0) = \int_{-\pi}^{\pi} \mathrm{d}\phi \, S_n(\phi, \theta|\phi_0, \theta_0).$$

Then

$$\begin{aligned}\mathcal{T}^0(u, \mathbf{k}_0) &= \cos\theta_0 \int_0^{\pi/2} \mathrm{d}\theta \, \sin\theta\sigma^0(\theta|\theta_0), \\ \mathcal{T}_n(u, w, \mathbf{k}_0) &= \cos\theta_0 \int_0^{\pi/2} \mathrm{d}\theta \, \sin\theta\sigma_n(\theta|\theta_0), \qquad n \geqslant 0.\end{aligned}$$

We can calculate the functions $\sigma_n(\theta|\theta_0)$ (which depend on u and w) explicitly, utilizing the formula

$$\int_{-\pi}^{\pi} \mathrm{d}\phi \exp(b\cos\phi) = 2\pi I_0(b) = 2\pi J_0(\mathrm{i}b),$$

where $J_0(\zeta)$ means Bessel's function of index zero. Thus, for $n \geqslant 1$,

$$\sigma_n(\theta|\theta_0) = \mathcal{T}^0(u, \mathbf{k}_0)\frac{w^2u^{2n}}{nn!}\exp\left(-\frac{w^2}{2n}\sin^2\theta_0\right)\exp\left(-\frac{w^2}{2n}\sin^2\theta\right)I_0\left(\frac{w^2\sin\theta_0}{n}\sin\theta\right). \tag{67}$$

(cf expressions (55) and (63).) After defining the dimensionless function

$$B(q,\theta_0) = 2q\cos\theta_0\exp(-q\sin^2\theta_0)\int_0^{\pi/2}\mathrm{d}\theta\sin\theta\exp(-q\sin^2\theta)I_0(2q\sin\theta_0\sin\theta), \tag{68}$$

we find that

$$\sum_{n=1}^{\infty}\mathcal{T}_n(u, w, \mathbf{k}_0) = \mathcal{T}^0(u, \mathbf{k}_0)\sum_{n=1}^{\infty}\frac{u^{2n}}{n!}B\left(\frac{w^2}{2n}, \theta_0\right). \tag{69}$$

In the special case of the perpendicular incidence (i.e. if $\theta_0 = 0$),

$$\begin{aligned} B(q,0) \equiv B_\perp(q) &= 2q\int_0^{\pi/2}\mathrm{d}\theta\sin\theta\exp(-q\sin^2\theta) \\ &= 2\sqrt{q}\exp(-q)\int_0^{\sqrt{q}}\mathrm{d}t\exp(t^2) = \sqrt{\pi q}\exp(-q)\mathrm{erfi}(\sqrt{q}). \end{aligned} \tag{70}$$

We recall that

$$\mathrm{erfi}(v) = \frac{\mathrm{erf}(\mathrm{i}v)}{\mathrm{i}} = \frac{2}{\mathrm{i}\sqrt{\pi}}\int_0^{\mathrm{i}v}\mathrm{d}t\exp(-t^2) = \frac{2}{\sqrt{\pi}}\int_0^{v}\mathrm{d}t\exp(t^2).$$

(We use the denotation $\mathrm{erf}(v)$ for the normalized error function, $\mathrm{erf}(\infty) = 1$.) If θ_0 is not equal to zero, integral (68) cannot be reduced analytically to a simple expression. Quite generally, however,

$$B(0,\sin\theta_0) = 0, \qquad \lim_{q\to\infty}B(q,\sin\theta_0) = 1. \tag{71}$$

To verify that $B(q,\sin\theta_0)$ tends to unity if $q\to\infty$, let us take $\sin\theta_0 > 0$, $\sin\theta > 0$ and utilize the asymptotic expression $I_0(v) \approx \exp(v)/\sqrt{2\pi v}$ [6]. So we obtain the integral

$$B(q,\theta_0) \approx \cos\theta_0\sqrt{\frac{q}{\pi}}\int_0^{\pi/2}\mathrm{d}\theta\sqrt{\frac{\sin\theta}{\sin\theta_0}}\exp[-q(\sin\theta-\sin\theta_0)^2].$$

However,

$$\lim_{q\to\infty}\sqrt{\frac{q}{\pi}}\exp[-q(\sin\theta-\sin\theta_0)^2] = \delta(\sin\theta-\sin\theta_0) = \frac{1}{\cos\theta_0}\delta(\theta-\theta_0)$$

and this proves the asymptotic property $B(\infty,\theta_0) = 1$ for all values of $\theta_0 \in (0,\pi/2)$.

In figure 1, we have plotted seven functions $B(q,\theta_0)$ distinguished by the parameter $\sin\theta_0$ for which we have chosen the values $\sin\theta_0 = n/8$ ($n = 0$ and $n = 2, 3, \ldots, 8$). For $q \approx 2$, the uppermost (full) line corresponds to the function $B(q,0) \equiv B_\perp(q)$ (the perpendicular incidence, $\theta_0 = 0$). The next full line shows the function $B(q, \arcsin(1/4))$; afterwards, the uppermost dotted line shows the function $B(q, \arcsin(3/8))$, etc. (The curve

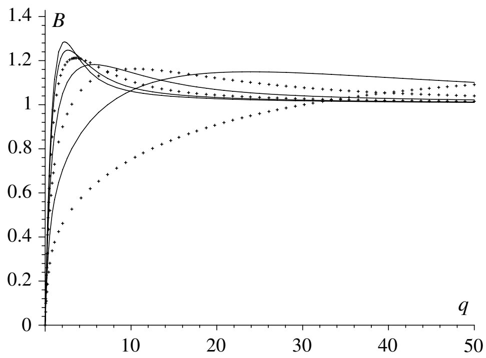

Figure 1. The function $B(q, \theta_0)$ for chosen values of θ_0. All the curves cross each other. For q approaching zero, the identification of the curves from above downwards is as follows: (*i*) the full lines correspond to the values of $\sin\theta_0$ equal to 0, 1/4, 1/2 and 3/4; (*ii*) the lines suggested by points correspond to the values of $\sin\theta_0$ equal to 3/8, 5/8 and 7/8.

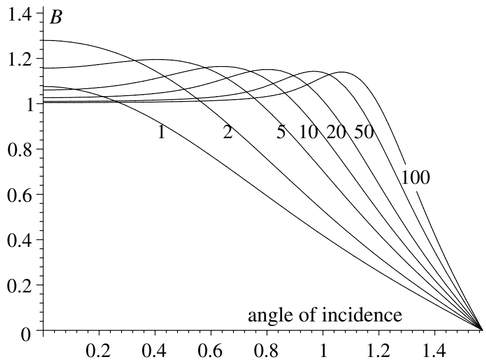

Figure 2. The function $B(q, \theta_0)$ for the values of q equal to the integers labelling the plotted curves.

for $B(q, \arcsin(1/8))$ has not been plotted since it would practically coincide with the curve for $B_{\perp}(q)$. The scale of figure 1 has not allowed us to show that the curve for $B(q, \arcsin(7/8))$ does also reach a maximum, as all other curves in figure 1 do.)

In figure 2, we have plotted seven functions $B(q, \theta_0)$, distinguished by chosen values of q. Figure 2 manifests that the dependence of $B(q, \theta_0)$ on the angle of incidence θ_0 is sensitive to the value of the parameter q.

Let us now highlight our main result. It is the explicit formula for the total tunnelling probability which reads:

$$\begin{aligned} \mathcal{T}(u, w, \theta_0) &= \mathcal{T}^0(u, w, \theta_0) + \sum_{n=1}^{\infty} \mathcal{T}_n(u, w, \theta_0) \\ &= \bar{\mathcal{T}} \exp(u^2)\left[1 + \sum_{n=1}^{\infty} \frac{u^{2n}}{n!} B\left(\frac{w^2}{2n}, \theta_0\right)\right]. \end{aligned} \tag{72}$$

Bearing this formula in mind, we can discuss how diffusive the tunnelling under consideration actually is. What we can say *a priori* is that the tunnelling is certainly not diffusive if $\ell \to \infty$

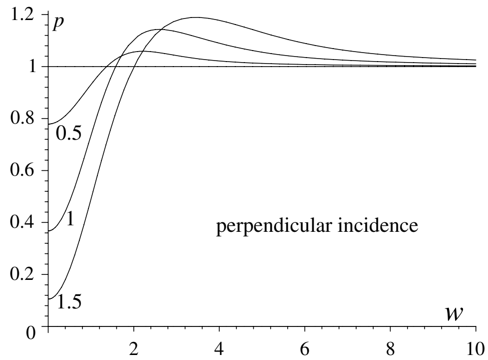

Figure 3. The function $p(u, w, \theta_0)$ with the constant parameters u and θ_0. (The curves have been calculated with $\theta_0 = 0$ and with u equal to 0.5, 1.0 and 1.5.)

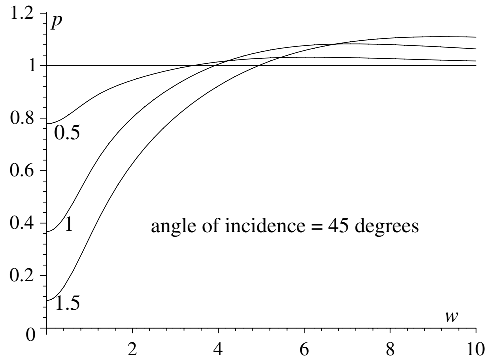

Figure 4. The function $p(u, w, \theta_0)$ with the constant parameters u and θ_0. (The curves have been calculated with $\theta_0 = \pi/4$ and with u equal to 0.5, 1.0 and 1.5.)

(i.e. if $w \to \infty$). Therefore, we deem it reasonable to focus attention on the ratio

$$p(u, w, \theta_0) = \frac{\mathcal{T}(u, w, \theta_0)}{\mathcal{T}^\infty(u, \theta_0)} = \exp(-u^2)\left[1 + \sum_{n=1}^{\infty} \frac{u^{2n}}{n!} B\left(\frac{w^2}{2n}, \theta_0\right)\right]. \tag{73}$$

In general, this positive function is partly greater and partly smaller than unity, as is shown in figures 3 and 4.

These illustrations show that if the values of u and θ_0 are kept constant, the quantity $p(u, w, \theta_0)$ is not a monotonous function of the variable w. There exists a critical value $w_c(u, \theta_0)$ (and correspondingly a critical value ℓ_c of the correlation length) given by equation

$$p(u, w_c, \theta_0) = 1. \tag{74}$$

Generally, we can state that

$$\begin{aligned} \mathcal{T}(u, w, \theta_0) &< \mathcal{T}^\infty(u, \theta_0) \qquad \text{if} \quad 0 < w < w_c(u, \theta_0), \\ \mathcal{T}(u, w, \theta_0) &> \mathcal{T}^\infty(u, \theta_0) \qquad \text{if} \quad w_c(u, \theta_0) < w. \end{aligned} \tag{75}$$

Let $w_{max}(u, \theta_0)$ be the value of w corresponding to the maximum value of $p(u, w, \theta_0)$. (Figures 3 and 4 suggest the existence of just one maximum for each depicted curve. All the curves approach unity from above if $w \to \infty$. The maximum point of the curve for

$p(1.5, w, \pi/4)$ lies at $w_{\max}(1.5, \pi/4) \approx 9.21$.) When comparing figure 3 with figure 4, one can conclude that $w_{\max}(u, \theta_0)$ is an increasing function of the angle of incidence θ_0. (Of course, $w_c(u, \theta_0)$ is also an increasing function of θ_0.)

5.2. *Dependence of the scattering matrix on the directional angles θ and ϕ*

For the forward scattering, the function $S(\phi, \theta|\phi_0, \theta_0)$ involves, according to formula (60), the sharp component $S_0(\phi, \theta|\phi_0, \theta_0)$ (proportional to $\delta(\phi - \phi_0)\delta(\theta - \theta_0)$) and the diffusive component

$$S^{\mathrm{dif}}(\phi, \theta|\phi_0, \theta_0) = \sum_{n=1}^{\infty} S_n(\phi, \theta|\phi_0, \theta_0). \tag{76}$$

The finiteness of the correlation length ℓ implies that $S^{\mathrm{dif}}(\phi, \theta|\phi_0, \theta_0)$, taken generally as a function of the angle of longitude ϕ and of the azimuthal angle θ, reveals a blurred distribution concentrated around the direction given by the angles ϕ_0 and θ_0. We will now discuss the significance of this angular blurring. Without loss of generality, we choose $\phi_0 = 0$. We focus attention on the function

$$\begin{aligned} P(u, w, \phi, \theta|\theta_0) &= \frac{S^{\mathrm{dif}}(\phi, \theta|0, \theta_0)}{S^{\mathrm{dif}}(\phi, \theta_0|0, \theta_0)} = \frac{S^{\mathrm{dif}}(\phi, \theta|0, \theta_0)}{S^{\mathrm{dif}}(\phi, 0|0, 0)} \\ &= \sum_{n=1}^{\infty} \frac{u^{2n}}{nn!} \exp\left(-\frac{w^2}{2n}(\sin^2\theta_0 - 2\sin\theta_0\sin\theta\cos\phi + \sin^2\theta)\right) \Bigg/ \sum_{n=1}^{\infty} \frac{u^{2n}}{nn!}, \\ &\quad 0 \leqslant \theta < \pi/2, \qquad -\pi < \phi < \pi. \end{aligned} \tag{77}$$

To illustrate this function graphically, we choose $u = 1$ and two typical values of the angle of incidence, $\theta_0 = 0$ and $\theta_0 = \pi/4$ (as in figures 3 and 4). If $\theta_0 = 0$, the function P is independent of the angle of longitude ϕ. Indeed,

$$P(u, w, \phi, \theta|0) \equiv P_{\perp}(u, w, \theta) = \sum_{n=1}^{\infty} \frac{u^{2n}}{nn!} \exp\left(-\frac{w^2}{2n}\sin^2\theta\right) \Bigg/ \sum_{n=1}^{\infty} \frac{u^{2n}}{nn!}. \tag{78}$$

(Owing to the denominator $\sum_{n=1}^{\infty} u^{2n}/(nn!)$ in (77) and (78), the functions P and $P_{\perp}$ are dimensionless and normalized. Note that $\sum_{n=1}^{\infty} \zeta^n/(nn!) = \mathrm{Ei}(\zeta) - \ln\zeta - \gamma$, where $\mathrm{Ei}\zeta = -\mathrm{v.p.} \int_{-\zeta}^{\infty} \mathrm{d}t \exp(-t)/t$ is the exponential integral and γ is Euler's constant: $\gamma = 0.577\,215\,6649\ldots$ [6].)

The function $P_{\perp}(u, w, \theta)$ is plotted in figure 5 for $u = 1$ and $w = 1, \ldots, 5$. The interpretation of figure 5 is simple: as the correlation length ℓ (and then the parameter w) grows, the blurring of the tunnelled beam gradually ceases to occur since if $w \to \infty$, the 'horizontal randomness' of the barrier height $V_0(\vec{\rho})$ ceases to be effective and there is no reason for any lateral scattering in the tunnelling. (Moreover, if $w \to \infty$, then generally the function $S^{\mathrm{dif}}(\phi, \theta|\phi_0, \theta_0)$ decreases to zero.) In figure 6, we show the same as in figure 5 for the oblique incidence with $\theta_0 = \pi/4$ and for the angle of longitude $\phi = \phi_0 = 0$.

6. Concluding remarks

In our calculations, we have assumed, in order to simplify some mathematical derivations, that the values of the parameter u should not be too high in comparison with unity. We have excluded the case when $u \gg 3$ from consideration. (In such a case, it would be necessary

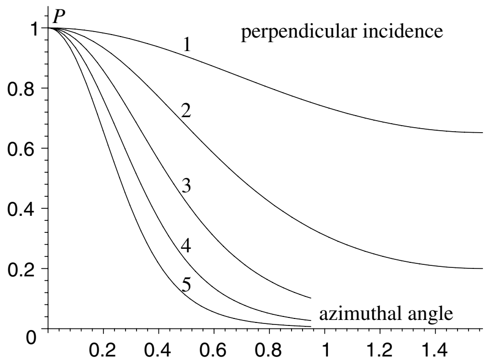

Figure 5. Dependence of $P \equiv P_{\perp}$ on the azimuthal angle θ for $\theta_0 = 0$ when the parameters u and w are given as constants. All the curves have been calculated with $u = 1$. The curves are labelled from above downwards by $w = 1, \ldots, 5$.

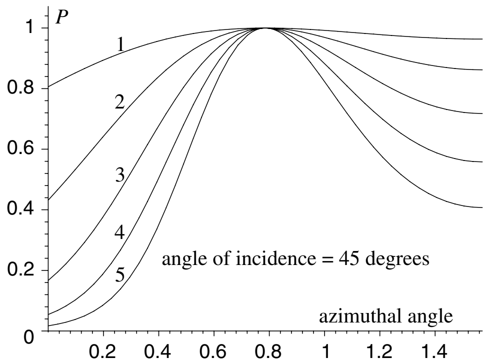

Figure 6. Dependence of P on the azimuthal angle θ for $\phi = \phi_0 = 0$ and $\theta_0 = \pi/4$ when the parameters u and w are given as constants. All the curves have been calculated with $u = 1$. The curves are labelled from above downwards by $w = 1, \ldots, 5$.

to average much more complicated functionals of the random function $V_0(\vec{\rho})$ than the simple exponential used in the present paper; cf expression (18).) However, when u is of the order of magnitude of unity, it is not a 'small' parameter. In this context, we are justified to accentuate that our calculations with $u < 3$ have not been 'perturbational' at all. If one of the coordinates x, y (say y) is chosen as a constant, the 2D plot of the barrier function $V_0(x, y)$ looks like a crest of mountains with randomly distributed saddles. We may interpret the correlation length ℓ of $V_0(x, y)$ as the average width of these saddles. The particles (in our case electrons), when impacting upon the barrier, prefer to tunnel across the barrier below the low-settled and wide enough saddles. However, the probability to find wide saddles among low-settled ones in a typical crest is very small. As we have shown (cf e.g. figure 3), the most efficient tunnelling is realized through barriers defined with the values of $w = k\ell$ which are neither too low nor too high.

In figures 5 and 6, we have shown the dependence of P on the azimuthal angle θ. In the case of the oblique incidence (figure 6, $\theta_0 = \pi/4$), it is also interesting to show how P depends on the angle of longitude ϕ. This dependence is presented in figure 7. (The distribution function $P(u, w, \phi, \pi/4|\pi/4)$ has been calculated according to formula (77) for $u = 1$ and for the same chosen values of w as in figure 6.)

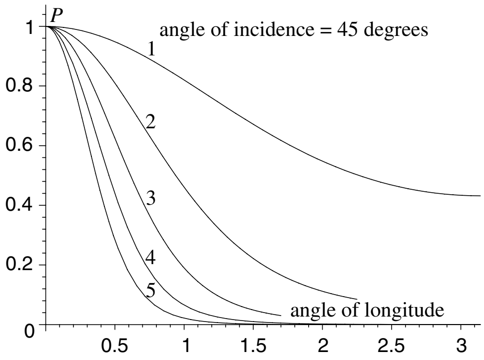

Figure 7. Dependence of P on the angle of longitude ϕ for $\phi_0 = 0$ and $\theta = \theta_0 = \pi/4$ when the parameters u and w are given as constants. All the curves have been calculated with $u = 1$. The curves are labelled from above downwards by $w = 1, \ldots, 5$.

We hope that our theoretical results may apply to some barrier structures incorporated in microelectronic devices. The solid-state literature is full of many examples of structures with tunnelling barriers. We believe that wherever the barrier height V_0 was hitherto approximated as a constant, it is always possible to realize a generalization and treat V_0 as a fluctuating variable. In a theoretical description of problems with fluctuating potentials, it is particularly advantageous to employ Feynman's path integrals [7]. The tunnelling through fluctuating barriers continues being interesting in its own right, although the fluctuations of the barrier height V_0 were often considered as a function stochastic in time (cf e.g. [8–10]). However, we have had in mind a different problem since we have considered barrier fluctuations in space. The generalization of the tunnelling theory in this sense necessitates the correct elucidation of the angular distribution of the tunnelling probability density and of the diffusivity of the tunnelling. This was with what we decided to deal in this article in detail.

The necessity to treat barriers with random heights was clear to investigators who interpreted currents across Schottky barriers within the framework of a classical thermionization theory [11–15]. In fact, electrons can traverse the Schottky barriers not only by jumping over them (thermionization) but also by tunnelling through them. This idea, when applied to deterministically defined Schottky barriers, was discussed by many authors. But then, the scheme of calculations that we have described in the present paper could surely be applicable to random Schottky barriers (although with a modification respecting the non-rectangular shape of the Schottky barriers).

As an exemplary experimental arrangement for which our calculations could apply directly, we can recall a metal–insulator–metal (MIM) structure [16]. In the simplest one-band theory of such a structure, $\psi(\mathbf{r})$ signifies the envelope wavefunction [17, 18] of the conduction electron tunnelling across the insulating layer which is considered as a potential-energy barrier. In the literature about MIM structures, V_0 used to be considered as a constant. However, the insulating layer I, but also the interfaces between I and M, may contain randomly distributed defects which necessarily imply the randomness of the potential energy of electrons inside the layer I, i.e. the randomness of the barrier height V_0 which was the basic assumption in the present paper. In particular, this randomness can be relevant in double-barrier configurations. It has long been well known that if two parallel deterministically defined barriers are located in a precise distance from one another, there are certain 'resonant energies' at which particles (say electrons) can be transmitted through these barriers with the probability approaching unity.

It is clear that this resonance behaviour can be broken if the barrier heights are stochastic. Therefore we believe that the theory that we have presented in this paper may be useful for quality assessments of resonant tunnel devices.

Here, however, we have also to mention another problem. In the last decade, many authors devoted attention to the resonant tunnelling in a quite different sense: namely to the tunnelling through localized states inside the barrier. For instance, a sandwich structure GaAs/AlGaAs/GaAs with a thin AlGaAs-interlayer may be viewed as a rectangular tunnelling barrier for electrons with a height V_0 determined by the Fermi energy and by the values of the forbidden gaps of GaAs and AlGaAs. If the AlGaAs-interface hosts impurity atoms or is disordered, there may exist localized states with energies $E_{\mathrm{i}} < V_0$ in it. (These energies can be identified as deep levels in the forbidden gap of AlGaAs.) If we realize the tunnelling at energies coinciding with (or being close to) E_{i}, we may speak of the resonance tunnelling (cf e.g. [19, 20]). (We may even consider, as recently Gryglas *et al* did [21], the 'phonon-assisted resonance tunnelling'.)

The resonant tunnelling in this sense has been a vital attribute in the explanation of the tunnelling magnetoresistance, a phenomenon that was observed with some thin-film tunnel junctions in which two ferromagnets were separated by a thin insulating layer (cf e.g. [22–24]). (In this case, one speaks of spin-polarized tunnelling.) Being aware of the importance of impurities and disorder for the tunnel magnetoresistance effects, Sheng *et al* and Los have recently published theoretical papers [25, 26] which are, we believe, complementary to ours. In [25], Sheng *et al* presented a theory of the impurity resonant tunnel magnetoresistance assuming the impurity potential inside the barrier in the form $V(\mathbf{r}) \sim -\sum_i V_i \exp(-|\mathbf{r} - \mathbf{r}_i|/\lambda)$. They have calculated the tunnelling conductance with $\lambda \to +0$ and with a constant barrier height. It would be interesting to generalize their approach and treat, as we have done it in the present paper, also barriers with randomly oscillating heights. We can say the same when commenting on [26]. The author of [26] has elaborated an extensive self-consistent theory of the scattering at disordered interfaces in layered nanostructures considering randomly distributed pointlike scatterers localized at interfaces. Los [26] draws also attention, among other ideas, to the significance of *roughness* of interfaces. If a rectangular barrier is rough, it means that its thickness a is a random function. Thus we may conclude that it is well possible to ascribe the diffusivity of the tunnelling—the aspect to which we have put the main attention in the present paper—not only to the randomness of the barrier height but also to the randomness of the barrier width. This kind of the randomness of a barrier can be accompanied, although not inevitably, with the randomness of the distribution of impurities and/or structural defects inside the barrier.

Acknowledgments

This work has been supported by the Slovak Research and Development Agency under the contract No. APVV-51-003505.

References

[1] Ziman J M 1979 *Models of Disorder* (Cambridge: Cambridge University Press)
[2] Landau L D and Lifshitz E M 1977 *Quantum Mechanics* 3rd edn (Oxford: Pergamon)
[3] Bezák V 2007 *J. Math. Phys.* **48** 112108
[4] Bezák V 2007 *Appl. Surf. Sci.* at press
[5] Bezák V 1970 *Proc. R. Soc. Lond.* A **315** 339
[6] Abramowitz M and Stegun I A 1964 *Handbook of Mathematical Functions (Appl. Math. Series* vol 55*)* (Washington D.C. Natl Bureau of Standards)

[7] Kleinert H 2004 *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets* 3rd edn (Singapore: World Scientific)
[8] Iwanishewski J 2000 *Phys. Rev.* B **61** 4890
[9] Ankerhold J and Pechukas P 2000 *Europhys. Lett.* **52** 264
[10] Goychuk I and Hänggi P 2005 *Adv. Phys.* **54** 525
[11] Tung R T 1992 *Phys. Rev.* B **45** 13509
[12] Tung R T 2001 *Mater. Sci. Eng.* R **35** 1
[13] Dobročka E and Osvald J 1994 *Appl. Phys. Lett.* **65** 575
[14] Dobročka E and Osvald J 1995 *Appl. Phys. Lett.* **66** 3069
[15] Osvald J and Dobročka E 1996 *Semicond. Sci. Technol.* **11** 1198
[16] Sze S M 1982 *Physics of Semiconductor Devices* (New York: Wiley-Interscience) chapter 4
[17] Ziman J M 1972 *Principles of the Theory of Solids* (Cambridge: Cambridge University Press)
[18] Callaway J 1974 *Quantum Theory of the Solid State* (New York: Academic) part B, chapter 5
[19] Knauer H, Richter J and Seidel 1977 *Phys. Status Solidi* a **44** 303
[20] Halbritter J 1982 *Surf. Sci.* **122** 80
[21] Gryglas M, Baj M, Chenaud B, Jouault B, Cavanna A and Faini G 2004 *Phys. Rev.* B **69** 165302
[22] Tsymbal E Yu and Pettifor D G 1998 *Phys. Rev.* B **98** 432
[23] Varalda J, de Oliveira A J A, Mosca D H, George J-M, Eddrief M, Marangolo M and Ergens V H 2005 *Phys. Rev.* B **72** 081302
[24] Garcia V, Jaffres H, Marangolo J-M, Eddrief M and Etgens V H 2006 *Phys. Rev. Lett.* **97** 246802
[25] Sheng L, Xing D Y and Sheng D N 2004 *Phys. Rev.* B **69** 132414
[26] Los V F 2005 *Phys. Rev.* B **72** 115441